

Dimethyl adipate
627-93-0 | DTXSID8025096

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.92e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.01e-01

Confidence level: 7.32e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Fumaryl chloride</div> <div>Measured: 6.04e-02</div> <div>Predicted: 1.29</div>	<div>Image not found</div> <div>Phenyl acetate</div> <div>Measured: 4.39e-02</div> <div>Predicted: 3.39e-01</div>	<div>Image not found</div> <div>8-Pentadecanone</div> <div>Measured: 1.61e-01</div> <div>Predicted: 1.58e-03</div>
<div>Image not found</div> <div>Ethyl acrylate</div> <div>Measured: 1.05e-01</div> <div>Predicted: 32.1</div>	<div>Image not found</div> <div>N-Methoxymethylamine</div> <div>Measured: 1.80e-01</div> <div>Predicted: 122</div>	